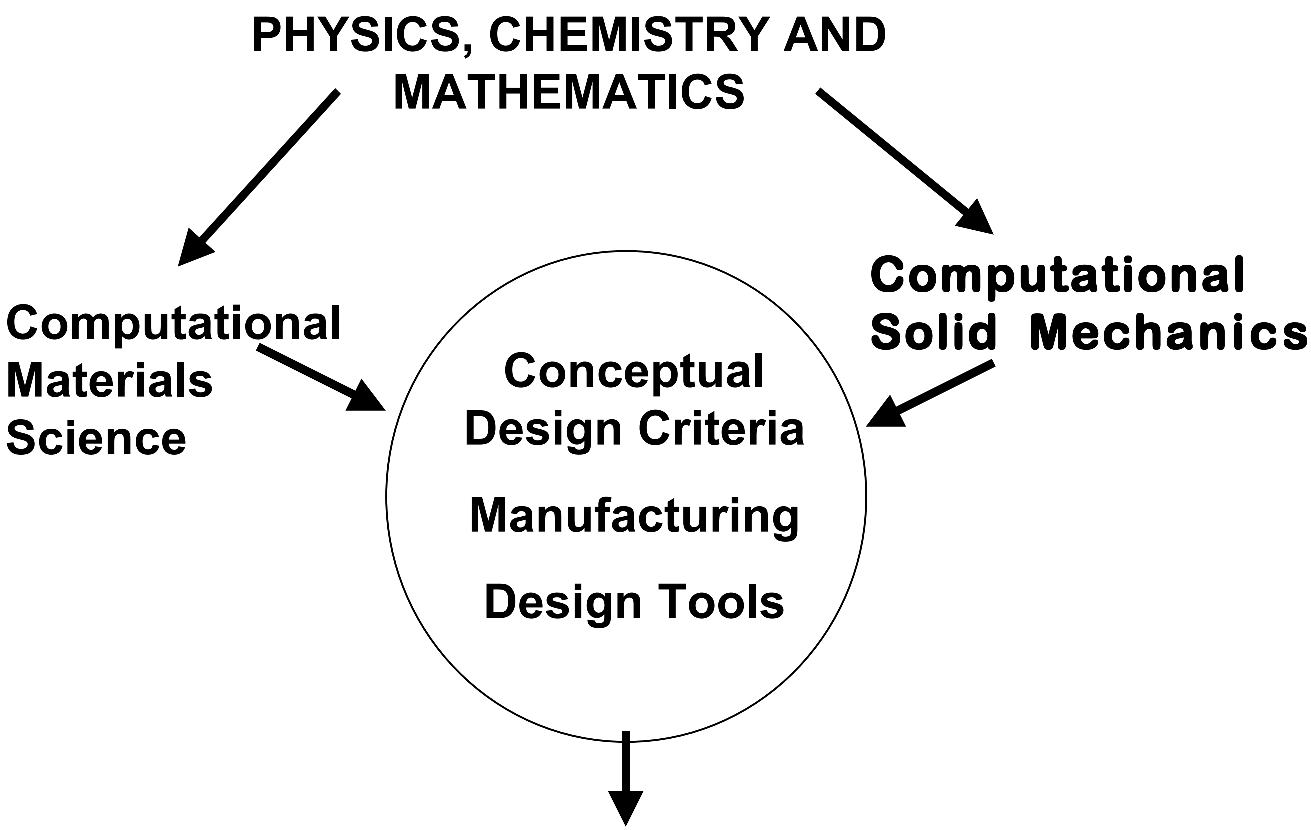
THE FACTORY-AFTER-NEXT

RAPID MANUFACTURING AT THE MESOSCALE

(10nm TO 2 mm)



MANUFACTURING, RELIABILITY AND FUNCTIONAL USE

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13. ABSTRACT *(Maximum 200 words)*

The objective of this workshop was to identify critical research directions required to achieve experimentally validated computational materials science and engineering. Currently, physics and chemistry-based models are useful for qualitatively predicting trends for optical, magnetic, and electrical behavior. However, they have marginal utility for predicting structural performance. The attendees noted significant progress in computational materials science. However, there was general agreement that projected increases in computing power are not in themselves sufficient to guarantee adequate materials modeling capability to meet future defense needs. Several areas were identified where additional theoretical and experimental work is needed. The importance of close coordination between theory and experiment was emphasized, as was the need for theoretical research to produce widely applicable computational tools for the scientific and engineering communities. Novel fabrication methods, such as self-assembly, layer-by-layer fabrication, and other fine-scale materials delivery and processing methods, were discussed, as were the importance of modeling processes such as nucleation, diffusion and microstructure formation. Emphasis was on microsystems in the 10 nm to 2 mm size range.

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Final Report

September 30, 1999

Rapid Manufacturing – "The Factory After Next"

***Robert A. Weller,** Vanderbilt University &*
***Robert R. Reeber,** U.S. Army Research Office*

Contract #DAAH04-96-C-0086

Robert A. Weller **Robert R. Reeber**

Foreword

On May 21, 1998, in remarks to the Armor Conference entitled, “Leadership is More Than Managing the Status Quo,” General Dennis J. Reimer, Chief of Staff of the U. S. Army, made the following statement.

> “Enhancing logistics will also be an important part of the Army After Next. I have said many times that there will not be a Revolution in Military Affairs until first we have a Revolution in Military Logistics. This means putting our faith in concepts like Velocity Management and Total Asset Visibility, giving up the comfort of stockpiling supplies on an iron mountain. We have to depend on systems that will deliver the right support, at the right time, at the right place. That bothers people -- that bothers me. I spent 28 years in an Army where the philosophy was that if anything went wrong we had two or three parts to replace it. We cannot afford that anymore. What we have got to do is invest in things that allow us to get the parts there on time, very quickly. We have got to build the systems that will give us the confidence and responsiveness we need - that is why the Revolution in Military Logistics is very important to us -- and a key, vital component of the Army After Next.”

The Army After Next is going to need “Factories After Next” to support it. From an articulation of need, through design and testing, to manufacture and deployment, the time to meet an unanticipated need of the Army must be measured in days, rather than weeks or months. In order to respond to a challenge of this magnitude, the processes of design, testing, and manufacture must be fully linked so that the time-consuming tasks of prototyping and testing can be reduced to a minimum.

Popular science fiction envisions a time when matter can be built up atom-by-atom by computers of transcendent complexity. Few would argue that such a thing will ever be physically possible, and yet in all good fiction there is a seed of truth. From today until the time of the Army After Next is about the same amount of time, approximately 20 years, as has elapsed from the first appearance of personal computers until today. As the GHz personal computer moves inexorably toward the living room, it is essential that we begin to assemble the foundation for the Factory After Next. Since materials are a necessary part of all manufacturing processes, we focus our attention upon them and, in particular, upon the computation of their physical properties.

Today, materials computation is intellectually fragmented, encompassing activities ranging from *ab initio* quantum mechanical computations at the microscopic scale to finite element analysis at the macroscopic scale, and including many specialized subjects. There are several high value-added areas such as drug design and semiconductor process and device modeling where aggressive development is underway for specific industrial objectives. However, comprehensive, scale independent modeling of generic low cost, low volume components, including variables affecting reliability and optimum properties such as microstructure, thermodynamic behavior, and other physical properties, is still very much a fragmented area of research.

Objectives

The objectives of this workshop were to establish the current state of the art in computational materials science and materials modeling and closely related experimental and process science, and to identify critical needs for scientific research, technological development, and validation. The emphasis was on the size range from approximately 10 nm to about 2 mm. This includes the crucial transition region between the atomic and the continuum scales and is appropriate to emerging micro-electro-mechanical system technologies (MEMS). Comprehensive, efficient, and reliable materials modeling, theoretically sound and experimentally validated, will be an indispensable engineering tool for the Factory After Next, and an essential element of the Revolution in Military Logistics envisioned by General Reimer.

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Executive Summary

The objective of this workshop was to identify critical research directions required to achieve experimentally validated computational materials science and engineering. Currently physics and chemistry-based models are useful for qualitatively predicting discovery trends for optical, magnetic and electronic behavior. In their present state of development they have marginal if any utility for designing and predicting the structural performance of working parts that address a designer's requirements for reliability at use temperatures and pressures.

Comprehensive, efficient, and reliable materials modeling based upon sound theoretical concepts and validated by laboratory experiments will be an indispensable engineering tool for the Factory After Next which will support future Army needs.

The emphasis of the meeting was on the size range from approximately 10ºnm to 2ºmm. This includes the crucial transition region between the atomic and continuum scales and is appropriate to emerging MEMS technologies. It is anticipated that new mesoscale fabrication methods will provide novel tailored experiments for rigorously testing finite element methods and first-principles theory.

The attendees noted the substantial progress that has been made in recent years in computational materials science, driven by rapid advances both in computer hardware and theoretical methods. There was, however, general agreement that projected increases in raw computational power in the foreseeable future are not, in themselves, sufficient to guarantee that adequate materials computation capability will be in place to support defense needs.

Several areas were identified where a lack of adequate theoretical understanding and not computational power limits progress. In general, these involve systems at high temperature or with excited states, where the local density approximation (LDA) fails. Engineers require design properties such as strength, thermal expansion, thermal conductivity, etc., while physicists have largely emphasized electronic and optical properties. Other challenge areas include microstructure evolution, non-equilibrium phase formation, phase diagrams of complicated compounds, corrosion, and the effects of size and geometry. In all cases, theoretical research should proceed hand in hand with appropriate validation experiments. Generally, this has not been the style of theoretical research funded in recent years.

An expected outcome of theory will be to supply validated inputs for relatively simple parametric models. These would be analogous to those now used for semiconductor process simulation. Such models must be seamlessly integrated into intelligent software and in-situ feedback manufacturing control systems that will handle decisions such as establishing the range of validity and selecting the appropriate computational algorithms. This will permit design engineers to concentrate on design, rather than on the idiosyncrasies of their tools.

Fabrication methods based on self-assembly, layer-by-layer fabrication, and other novel fine-scale materials delivery and processing methods are seen as crucial in the size range of interest. These, now the subjects of aggressive laboratory research, involve precisely the processes, such as nucleation, diffusion control, and microstructure formation, for which theory is least satisfactory. Therefore, a key endeavor will be to design experiments complemented by theoretical or model predictions, so that the two converge rapidly. Strategic research policy should encourage this convergence and also mandate the delivery of general-purpose computational tools and algorithms as products of theoretical research. It is expected that such policies will positively stimulate commercial vendors who package, sell, and support the computational tools that are the most useful to materials and design engineers.

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Introduction

Robert R. Reeber
Materials Science Division
U.S. Army Research Office

In September of 1997, I was asked to review rapid prototyping developments for an international research coordination meeting. In preparing for the talk I found that the field relies primarily on empirical methods, (i.e. robotically-controlled scribe needles or laser interferometric methods to convert a costly machined part's surface into a 3D computer-aided design or CAD file). The elimination or at least minimization of machining costs provided a significant incentive for such CAD-CAM manufacturing. In my talk I related research results from nanoscale fabrication of high strength refractory metal weaves to what I thought might be achieved with future advances in electron (E-beam) processing of materials.

The purpose of this workshop is to identify technical trends that, additional to reducing machining costs, can lead to designed-in structural reliability of rapidly manufactured components. This would require something more than just empirically generated CAD-CAM files. In contrast to a silicon factory we envision a broader product line that produces smaller runs of product, utilizes significantly more materials compositions and part geometries and provides MEMS products that can operate at adverse temperatures and pressures.

One can envision objectives that include:

1). Significant improvements to provide computational modeling for generating CAD/CAM files.

2). Utilization of computer controlled processes that have sufficiently high resolution to yield control of component microstructure.

3). Provisions for in-situ diagnostics to monitor and control the manufacturing process.

Perhaps, with the experience of the computer revolution to draw on, it might be expected that the first applications of such technology are on the meso/microscale or MEMS and directed toward relatively high value added products. Ashby, in his book, Materials Selection in Mechanical Design,[1] discusses the interactions between materials and shape in detail at the macrolevel. He puts the need for appropriate design eloquently, "Today with more materials than ever before, the opportunities for innovation are immense. But advance is possible only if a procedure exists for a rational choice." Here we are looking for new means to expand the processing choices available and to improve existing processes for the regions he refers to as nano and microbeam technology.

[1] M.F. Ashby, Materials Selection in Mechanical Design, Pergamon Press, Oxford, UK , 1992.

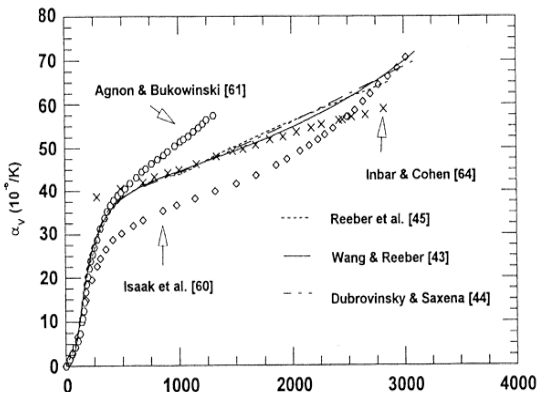

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Figure 1

Thermal Expansion of MgO

At these scales, many materials modeling efforts have been effectively operating in their own sandboxes with no verification of their efficacy. In spite of that one can foresee the developing integration of materials theory, computation, materials design and the manufacturing process.

In lieu of a better terminology we can call this rapid or “smart” micro-manufacturing. Some existing process technologies, as discussed later, have the potential for providing sufficient resolution or “manufactured BYTE sizes” with computer-aided control of microstructure.

Currently the state of the art in CAD file generation provides good external shape while only incidentally impacting internal quality. No optimization methods of materials properties for a given application are generally available. In future one must expect that introducing improved and efficient computational modeling that has been validated and verified will lead to designed in reliability.

Computational materials modeling currently has many problems. First principle physics calculations have been very successful in providing directions for electronics and optics research and developments. They unfortunately provide ground state or zero kelvin calculations and do not have good procedures for handling temperature effects due to anharmonicity and thermally induced defects. As we have discovered in our own work,[2] semi-empirical models based on simple lattice dynamical models offer significantly improved analytical expressions for thermal expansion. Figure 1 illustrates the difficulties theoretical approaches have in predicting the thermal expansion of MgO, a simple ionic solid.

Molecular dynamics offers good guides for chemical processes but requires realistic chemical potentials which are effectively non-existent for engineering materials especially when temperature, pressure and strain are variables. Grain averaging approaches (i.e. new statistics, finite element and finite difference methods) are in their infancy especially where anisotropic effects are important. Model predictions need to be verified at the component level. Too often modelers provide solutions to special problems that have minimal real world interest. A good example of how some of these concerns

[2] K. Wang and R.R. Reeber, The Role of Defects on Thermophysical Properties: Thermal Expansion of V, Nb, Ta, Mo, and W, Mat. Sci. and Eng. **R23**, 101-134, 1998.

are being approached is provided by the ARO-DOD-NSF-steel industry consortium program with Olson at Northwestern University.[3] Additional problems relating structure to materials properties include the following:

1. Models that accurately predict single crystal physical and mechanical properties as a function of T, P, X.
2. Models that include anisotropy, residual stresses and compositional effects in polycrystalline materials and predict physical and mechanical properties of manufactured components.
3. Improvements of and new innovations in computer-aided manufacturing that increase resolution and control of the manufactured "byte".

A key concern, after a materials model predicts properties and provides the ideal microstructure and gradient composition of a component, is to have the process control and resolution that allows actual manufacture of the specific component configuration.

The materials engineer relates microstructure to component properties. Important materials processing conditions must consider the following:

1. Phase transformation control/theory
2. Morphology control-grain size, distribution and orientation
3. Gradient coatings-compositional controls
4. Non-equilibrium coatings/materials
5. Thin (10-150 micron) to thick (1-2mm)
6. Structural stability

As mentioned briefly earlier, some processes, shown in Table 1, are available to provide part of the manufacturing capability imagined.

TABLE 1
Manufacturing

MESOSCALE	MICRO/MACROSCALE
• **Self - Assembly**	• **E-Beam Manufacturing**
• **Ink-jet Printing**	• **Photolithography & Sol Gels**
• **Nanolaminate CVD**	• **Plasma**
• **Ion Beam/Laser Ablation**	• **Torches/Laser Methods**
• **MEMS**	• **In situ control of Microstructures**
• **Soft Lithography**	• **What Else?**

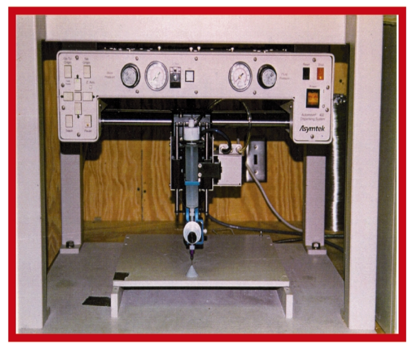
[3] G.B. Olson, Computational Design of Hierarchically Structured Materials, *Science* **277**, 1237-42, 1997.

Materials processed to date have included beta-silicon carbide, Ti, Al, Si. And Zr through laser pyrolysis, selective laser sintering and selective laser reaction sintering. Green ceramic parts from selective laser sintering can be hot thermally processed and infiltrated. A variety of glass ceramics, composites and metal parts have been processed with reactive stereodeposition, 3D printing, electron beam, electroplating, sputtering and selected area chemical vapor deposition (CVD) and MOCVD. Most of these methods have been developed through DOD with DARPA providing several large thrusts in metal and ceramics processing technology. The continuing challenge is to improve the manufacturing resolution and still provide cost-effective processes.

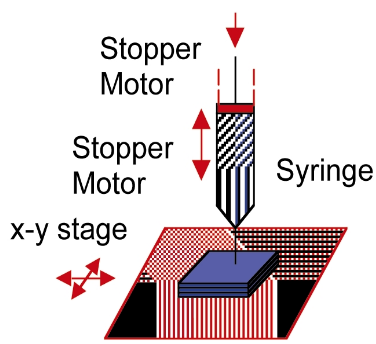
Figure 2 illustrates ARO-funded work at the University of Arizona on extrusion freeform fabrication where an "inkjet" printer deposits a sol gel material under computer control. The resulting preform is postprocessed into a ceramic. Gradient materials can be manufactured by using coextrusion of several materials or by depositing different composition layers. Sandia Laboratory has adopted and is commercializing some of this technology.

Other examples of mesoscale processing are provided by the ARO-DOD Multiuniversity Research Initiative at Princeton/Harvard/Drexel Columbia. Figure 3 illustrates the Whiteside group's work on controlled crystal growth by the lithographic printing of preferred orientation sites. A polymeric stamp provides a soft lithographed mark on a substrate which preferentially interacts with a surface active molecule (SAM) to provide for the controlled deposition of single crystal arrays of calcite.

Figure 2
EXTRUSION FREEFORM FABRICATION
(Paul Calvert - University of Arizona)



Asymtek fluid Dispenser used for extrusion freeforming.



Reactive Extrusion Freeforming

Figure 3
CALCITE CRYSTALS ON PATTERNED SAMs
GEORGE WHITESIDES
HARVARD UNIVERSITY

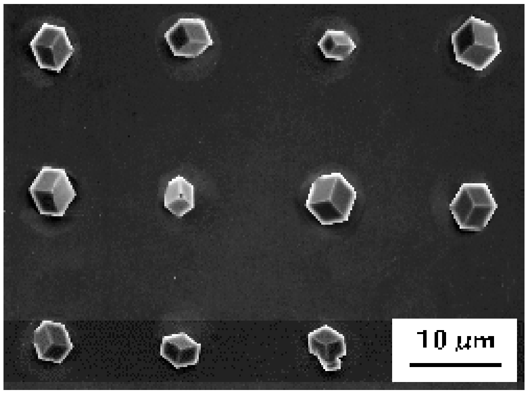
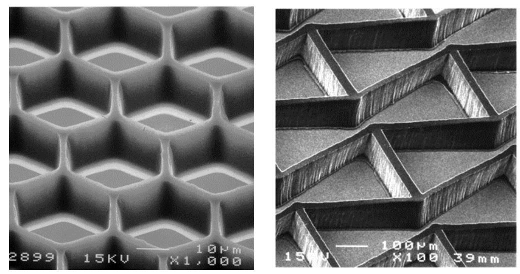


Figure 4 shows two dimensional negative Poisson's ratio structures that expand perpendicular to the tensile direction when pulled. These were made with similar techniques.

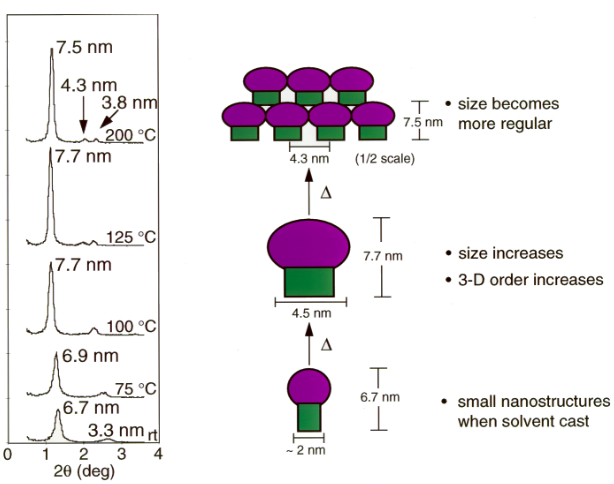
Figure 4
NEGATIVE POISSON'S RATIO MATERIALS
GEORGE WHITESIDES
HARVARD UNIVERSITY

µHoneycomb -- Carbon



An ARO project at the University of Illinois takes the design process one step closer to the chemical molecular level. The computer designed structures illustrated in Figure 5 have been experimentally synthesized and hierarchially stacked in the laboratory as illustrated by the x-ray scattering results. Initially we expect that the approach of introducing materials modeling directly in the design process will by necessity be applied at the meso/microscale for high-value-added smart systems.

Figure 5
University of Illinois-Stupp



Can we foresee some of the future trends in this technology? One would expect rapid manufacturing to eventually be optimized through the introduction of verifiable computational materials modeling. Such optimization would provide high reliability parts at the mesoscale in a five to ten year time frame. With automation and process developments, major property improvements and microstructural controls for larger parts should follow. Although not a reality as yet, futuristic articles and some new Defense research programs are scratching at the surface of this new area. The promise is to have designed-in reliability and optimum performance in addition to the convenience of computer-aided design of the shape of a part. But it is important to reiterate that the two primary requirements for success are:

1. The development of improved and verifiable materials modeling and

2. Providing complete control of "processing bytes" such that each process operation affects the structure and morphology of the part in a known and reproducible way.

COMPUTATIONAL MATERIALS SCIENCE AND MODELING

The successes of Computational Materials Science are concentrated on a fairly small selection of properties, most of them electronic or thermodynamic. There is still a wide gap between the type of information that first-principles calculations can produce and many of the properties materials engineers want. The direct output of first-principles calculations are energies, band structure, charge density, crystal constants, bond lengths, etc. While these are important properties, they are often difficult to relate to more macroscopic (but technologically relevant) properties, such as strength, corrosion resistance, creep, crystal structure, microstructure, transformation temperature and kinetics, etc. Building a link between electronic structure methods and macroscopic "engineering" information, remains one of the foremost challenges of Computational Materials Science.

The problems with quantitative property theories are often thought of as time and length scale problems, but really could be considered more as *knowledge* problems. To coarse-grain length and time, one needs to know what the relevant variables and processes are at each length or time scale. The focus of computational materials science should be on developing such property theories. While faster computers are always useful, the strong emphasis (almost unique emphasis) from some agencies on computational power and mathematical algorithms is misplaced. This is not the bottleneck, except for a small set of applications.

With computing power becoming less of an obstacle, computational materials science still has a large need for quantitative materials theories in order to apply what is found from atoms and electrons to macroscopic properties. This requires replacing the qualitative theories that are now common in materials science. Ironically, this is an area where the field of first-principles modeling can probably get a lot of help from experimentalists.

A major aspect of this workshop was how computational modeling can be used to predict material response and properties, such that current manufacturing capabilities can be significantly improved. For this to be accomplished, the appropriate scale at which computations are performed should be determined. There were presentations that described computations that ranged from the atomic to the continuum scales. Participants felt that a multiscale approach should be undertaken in which *dominant* mechanisms, properties, and failure modes are identified at each scale. In the computational field, tremendous efforts are being expended to determine how scaling relations should be obtained. However, these scaling relations should not be the main focus for the development of new materials or for improved manufacturing capabilities. Current efforts should be focused on the development and prediction of material properties at the appropriate levels. *Ab initio* computations can be used to obtain properties, such as band energies, crystal structure, etc. At longer scales, emphasis should be on obtaining estimates of the fracture and strength response of aggregates that are representative of realistic microstructures that exhibit characteristics, such as grain-boundaries, anisostropic crystalline structure, and interfacial and bulk energies.

Another important issue is how to tailor and optimize processing, interfaces, interphases, grain boundaries, and graded regions in heterogeneous materials for desired and optimal multi-functional applications. Most computations at the continuum level are based on homogenization techniques and Taylor-like models that smear out complex but essential details associated with physically realistic microstructures. There has to be a quantification, perhaps utilizing new or improved statistical methods, of the effects of different heterogeneities on overall performance and reliability.

Reliable and accurate computational predictions are needed to improve life-cycle estimates that account for variabilities in design and other uncertainties, to investigate what-if failure scenarios, and to gain insight into processes that would be difficult or impractical to measure. Experiments and prototype development are expensive, and cannot provide accurate predictions of phenomena, such as subsurface damage, high pressure failure initiation, and crack nucleation.

Several broad classes of problems may be categorized as follows:

I. Quasimacroscopic 'Engineering' equations adequately model the phenomena of interest; the needs are to solve these equations in a wider variety of situations and to obtain parameters from microscopic calculations. Some examples include:

   a. Near equilibrium thermodynamics
   b. Fracture
   c. Plasticity
   d. Diffusion
   e. Conventional hydrodynamics

   Specific needs that can be addressed here are:

   A. Obtain improved 'microscopic' understanding of:

      a. The whens and whys of Local Density Approximation (LDA) code failures; and LDA accuracy for specific calculations.
      b. High temperature. Highly excited states are not well understood, since LDA codes treat the ground state.
      c. 'Strongly correlated' systems.
      d. Situations where the Born-Oppenheimer approximation fails.
      e. Non-symmetrical conditions (Boundaries, anisotropy, etc).
      f. The adequacy of atomistic calculations. More detailed testing is required.

II. ‘Engineering‘ equations are not adequate. Here better quasimacroscopic representations are required. Some examples include:

  a. Morphology and kinetics of microstructure including shape, growth, size, density of grain boundaries.

  b. The consequences of microstructure on properties (mechanical, thermodynamic, electrical, etc.).

  c. Nonlinear aspects of diffusion.

  d. Corrosion.

  Their recommended needs include studies to provide a better understanding of:

  a. Coarse graining

  b. Effects of randomness on properties

Other Specific Observations and Recommendations:

1. Computer codes are publicly funded documents and should be available to all. Appropriate emphasis should be given to building tools not just writing special-purpose or idiosyncratic computer programs. Computer code is a form of publication, and every publicly funded computational project should contribute to the development of robust public-domain modeling tools. Publicly available codes need to be well documented, robust and user friendly. Agencies should include requirements in grants for code access by others and encourage platform independence and standard I/O. Achieving this will generally require a cultural change among computational scientists, who now often view codes as proprietary and do not view them as important end products of their research.

2. The community needs to realistically assess the success of basic physics and materials science in calculating and predicting the properties of solids based upon underlying atomic-scale physics.

3. We should press forward with the development of scaling theories to relate different levels of understanding and calculate the parameters in continuum theories from various branches of engineering. Overall, emphasis should be on microscopic science that enables quantitative materials modeling. The experience of the semiconductor industry with device and process modeling is instructive.

4. Challenge areas include:

   a. Microstructure evolution

   b. Non-equilibrium phase formation

   c. Phase diagrams of complicated compounds

   d. Corrosion

   e. Size and geometry effects

5. Theory has drifted apart from experiment and manufacturing, and there must be more communication in the future.

6. Today's unsolved problems involve non-equilibrium, non-linear, dynamic phenomena sensitive to atomic scale phenomena.

7. The most probable primary outcome of theory will be relatively simple parametric models and look-up tables that can be employed by manufacturing process engineers in order to control, design and modify industrial processes.

8. Both experiments inspired by manufacturing experience and experiments inspired by abstract theory are needed.

9. Dissemination of information and education: Computational modeling is an under-used tool in materials science and engineering. This is largely due to its rapid development and the concomitant lack of education on the topic in traditional MS&E programs. Most professional engineers have no education in this area and can not, therefore, evaluate the possibilities or limitations of computational modeling methods.

EXPERIMENTAL SCIENCE FOR MESOSCALE MANUFACTURING SUMMARY

The objectives here are to identify basic experimental research issues of relevance to flexible, rapid manufacturing. Of special interest are problems that occur as the scale of the part is reduced enough so that surface energy effects on processes become as important or in some cases more important than volume energy effects. As parts become smaller, more complex in chemical composition, and have feature sizes approaching diffusion lengths, it is essential to have design and manufacturing tools that insure long term reliability and reduce the costs of manufacturing. The complete empirical characterization required for high value added components such as those produced in a state-of-the-art silicon foundry is cost prohibitive for small batch lots of a wide range of MEMS systems.

New methods for non invasive, *in situ* diagnostics and programmed real time control of microstructure will be essential for controlling and optimizing specific component properties while obtaining improvements in reliability. Such needs are summarized in Section I of Table 1. Real time nondestructive evaluation of microstructure and phase stability from electronic and magnetic measurement techniques during manufacturing need to be developed and demonstrated. These, combined with improved solid state computations, can assist in interpreting microstructural status during manufacturing and service. Possibly the susceptibility to form sigma phase in superalloys, which is now determined by electron vacancy number calculation, can be measured using a combination of electronic and magnetic measurements.

Joining is an essential part of the manufacturing process. Each specific low temperature solid state bonding process needs to be understood and modeled to assist in the selection of its process parameters and consumables (coatings). Methods to accelerate the low temperature solid state bonding process, such as transient liquid phases, self-propagation (combustion) synthesis, and/or ion implantation of surfaces to be joined, need to be investigated and modeled to determine the process parameters. New techniques such as magnetic pulse joining need to be evaluated to demonstrate the ability to make dissimilar joints with various materials and part morphologies. Nondestructive methods need to be refined to assure the quality of reduced size joints in complex geometries.

In recent years many materials modeling efforts have been detached from experiment and have had only qualitative verifications of their efficacy. In rapid or "smart" manufacturing theories, models, and tools must be quantitatively validated by carefully chosen experiments. Some of the more important of these are listed in Section II of Table 1.

Some existing process technologies that have potential for providing sufficient resolution or "manufacturing BYTE sizes" and computer-aided control of microstructure include:

a. Polymers – Photolithography and sol gels.
b. Ceramics - Laser Pyrolysis & Photolithography Vapor Infiltration CVD, MOCVD.
c. Metals - Metal Spray, CVD, Sputtering, Electroplating, Laser.
d. Self assembly, ink jet printing.

Extensions of these and new layer-by-layer processes are required that can significantly reduce machining costs of refractory metal and ceramic parts.

Processes should be versatile enough to utilize fine scale gradient composition materials, gradient microstructures, and optimized micro-geometry, so that optimal capability and reliability are achieved. This puts additional demands on the controllability aspects of processing methods, as they must have narrow grain size distributions that are either frozen in place or capable of uniform modification. This would include knowing how to tailor and optimize heterogeneous material combinations for desired and optimal multifunctional applications so as to control effects and phenomena related to processing caused by interfaces, grain boundaries, and graded regions. Kinetic controls offer the flexibility of microstructure selection but also present significant challenges to process modeling.

A significant area for selected validation/verification information relates to non-equilibrium situations. Nucleation reactions expose a variety of kinetic preferences involving different metastable solids and microstructural options. As the materials choice widens, the need to understand and control stability and kinetic pathways of dissimilar materials will require a range of new barrier films as well as improved understanding of long term processes occurring in service. Validation/verification of a nucleation controlled reaction microstructure model requires specific data on melt undercooling (supersaturation), nucleation kinetics (statistics), interface velocity, thermal solutal history and some reasonable understanding of appropriate metastable phase diagrams. Advances are related closely to the availability of thermodynamic analysis, measurements for stable and metastable phase equilibria and the kinetics of reactions. The long term investment in nurturing the enabling knowledge base and carrying out key experiments that confirm empirical and semiempirical correlations of information is essential for making seamless advances in manufacturing. A key endeavor will be to carefully design complementary sets of data and modeling predictions so that the two converge with increasingly quantitative predictions.

TABLE 1

Experimental Science for Mesoscale Manufacturing
I. METHODS:
a. Real-time, non-invasive, in situ diagnostics
b. Programmed, real time, control of microstructure, composition, and geometry to achieve specific properties
c. Application of new in situ diagnostic tools i.e. tabletop high intensity x-ray sources, laser spectroscopy, etc.
d. Micromanipulation and microassembly robotics at smaller dimensions
e. Nondestructive inspection at small scales
II. CRYSTAL/ALLOY/COMPOSITE EXPERIMENTAL DATA FOR VALIDATION/VERIFICATION OF THEORIES/MODELS/TOOLS
a. Process Kinetics measurements
b. Residual Stress Measurements
c. Diffusion and thermodynamics data for multicomponent system analysis
d. Mechanical property measurements at MEMS scale (toughness, fracture, strength)
e. Welding and Joining (cold and warm) adhesion/interface properties and energies
f. Effects of anisotropy, grain orientation, residual stresses and non-equilibrium conditions
g. Measurements related to hydrodynamic properties: solidification, liquifaction, viscosity, surface tension, orientation, impurity composition
h. Effects of decreasing sizes and changes in geometry on all properties
III. OTHER NEEDS
a. Thin film microstructures evolution
b. Manufacturing using biomimetic principles i.e., graded and heterogeneous composites
c. New processing methods that allow improved resolution and part detailing, other innovative processes and ???
d. Low cost processing methods i.e., self assembly
e. Multicomponent phase diagram studies by combinatorial analysis

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WORKSHOP PROGRAM

RAPID MANUFACTURING - THE FACTORY AFTER NEXT

Co-sponsored by: The U.S. Army Research Office and Vanderbilt University
Workshop Chairs: Robert R. Reeber, ARO and
Robert A. Weller, Vanderbilt University, School of Engineering

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MONDAY MORNING
DECEMBER 14, 1998
Robert Weller, Vanderbilt University - Session Chair

8:00 a.m.	Registration (Room 118, Sarrett Student Center)
8:30 a.m.	Welcome - Robert Weller, Vanderbilt University
8:35 a.m.	Opening Remarks - Robert Reeber, U.S. Army Research Office
9:00 a.m.	*Computational Solid Mechanics and Prediction of Failure Initiation and Evolution* - Mohammed Zikry, North Carolina State University
9:35 a.m.	*Computational Materials Science: From Atoms to Macroscopic Properties* - Sokrates Pantelides, Vanderbilt University
10:10 a.m.	Break (catered)
10:40 a.m.	*Computational Materials Science and the Design of Novel Materials* - Gerbrand Ceder, The Massachusetts Institute of Technology
11:15 a.m.	*First Principle Models for Materials and Limits of Current Approaches for Materials Property Predictions* - Andrew Millis, Johns Hopkins University
11:50 a.m.	Lunch - (The University Club)

MONDAY AFTERNOON
DECEMBER 14, 1998
Sokrates Pantelides, Vanderbilt University, Session Chair

1:00 p.m.	*Chemical Potentials and Computational Materials Science* - Donald Brenner, North Carolina State University
1:35 p.m.	*Applying Finite Element Methods for Modeling Quantum Phenomena in Thin Films and Quantum Wires* - Harley Johnson, Brown University
2:10 p.m.	*Computational Materials Science and Atomistic Models of Fracture of Materials* - Michael Marder, University of Texas at Austin
2:45 p.m.	*New Statistical Approaches for Predicting Polycrystalline Microstructures of Materials* - Chuanshu Ji, University of North Carolina at Chapel Hill
3:20 p.m.	Break (catered)
3:50 p.m.	*Mesoscale Fabrication: Lessons From Electronic Device and Process Simulation* - Ronald Schrimpf, Vanderbilt University
4:25 p.m.	*Compliant Mechanism Based Manipulator Design for Micromanipulation and Microassembly* - Michael Goldfarb, Vanderbilt University
5:00 p.m.	Discussion
6:00 p.m.	Dinner - (The University Club)

TUESDAY MORNING
DECEMBER 15, 1998
Kamel Salama, University of Houston, Session Chair

8:30 a.m.	*Rapid Prototyping Technology, Lasers and Near Net Shape Processing of Materials Through Desktop Manufacturing* - Joseph Beaman, The University of Texas at Austin
9:05 a.m.	*Practical Considerations for Designing Ultra-Large Software Systems* - Gabar Karsai, Vanderbilt University
9:40 a.m.	*Fundamental Physical Considerations in Mesoscale Processing of Materials* - Leonard Feldman, Vanderbilt University
10:15 a.m.	Break (catered)
11:20 a.m.	*Thermodynamics, Kinetics and the Synthesis of New Materials* - John Perepezko, University of Wisconsin at Madison
11:55 a.m.	Lunch - (The University Club)

TUESDAY AFTERNOON
DECEMBER 15, 1998
James W. Mayer, Arizona State University, Session Chair

1:00 p.m.	*In situ Diagnostics for Thin Film and Surface Processing* - Eric Chason, Brown University
1:35 p.m.	*Mechanical Testing and Properties - Designing Ideal Micron Scale Mechanical Test Specimens* - William Sharpe, Johns Hopkins University
2:10 p.m.	*Novel Joining Techniques for Advanced Materials* - David Olson, Colorado School of Mines
2:45 p.m.	Break (catered)
3:10 p.m.	*Laser Near-net Shaping for Rapid Manufacturing - Potential for Mesoscale Structures* - William Hofmeister, Vanderbilt University
3:45 p.m.	*Freeforming and Biomimetic Materials* - Paul Calvert, The University of Arizona
4:20 p.m.	Discussion (catered)
7:00-10:00 p.m.	POSTER SESSION and DISCUSSION - (The University Club - Hot Hors d'oeuvres and Open Bar)

WEDNESDAY MORNING
DECEMBER 16, 1998
Robert Reeber, ARO, Session Chair

8:30 a.m.	Robert Reeber Charge to Panels
8:40 a.m.	Panel Meetings
10:30 a.m.	Break (catered)
10:50 a.m.	Panel Reports
11:50 a.m.	Critical Analysis and Summary
12:15 p.m.	Adjournment
12:15 p.m.	Lunch (no host)
	LAB TOURS BY ARRANGEMENT

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Organizers' Perspective of the Meeting

A diverse group of engineers and physical scientists was brought together to provide different insights on the role of computational materials modeling for the design of robust mesoscale materials systems. The group involved theoretical and experimental mechanics, as well as computational materials specialties (Zikry, Johnson, Marder, Sharpe, Ceder, Brenner, and Salama), theoretical physicists (Millis and Pantelides), mechanical engineers (Beaman and Goldfarb), process researchers (Calvert and Hofmeister), experimental materials scientists (Perepezko, Olson, and Chason), semiconductor materials and device researchers (Schrimpf, Feldman and Mayer), a statistician (Ji), a software engineer (Karsai) and the organizers (Reeber and Weller). Several invited speakers (Aksay, Fuller and Carter) involved with self-assembly processing and thermodynamic approaches to modeling microstructure were not able to attend. A major underlying theme was to identify roadblocks for efficient manufacturing at the mesoscale (2nm to 2 mm) of optimized property and affordable cost components. In that context, speakers addressed areas such as the feasibility for utilizing specific joining processes at the mesoscale, problems with testing and verifying bulk properties for very small specimens, in-situ diagnostics during processing, and the current use of modeling and theory to give qualitative estimates for some desired properties. The last topic has also been more fully documented in a recent Science article by Ceder.[1]

Talks on semiconductor and rapid prototyping manufacturing gave insights into what analogous problems might be expected as the part scale shrinks. Concerns were voiced regarding the lack of experimental inputs to theoretical predictions. Although critical data needs seem to limit the validity of theoretical predictions, it was also observed that this paucity of theoretical/experimental interactions prevented identification of key experiments that could quantitatively test theory. Additionally, there appeared to be serious inadequacies in macroscopic models for diffusion, mechanical properties and thermal properties.

Several of the speakers illustrated work relating to obtaining reproducible experimental results at smaller and smaller scales. Most of the theoretical work, with a few exceptions, related to electronic/optical/magnetic materials where theorists were looking for publishable discovery trends rather than at quantitative *structural* property predictability. Design and manufacturing engineers found such trends to be of minimal value for designing reliability and improving manufacturability. Examples cited from the semiconductor industry showed manufacturing problems solved by empirically and laboriously developing algorithmic solutions for each specific process. A general consensus was that manufacturing engineers did not have confidence in the near term development of robust theoretical models for manufacturing, but did look for and find useful fundamental inputs that helped them improve parameterized process characterization.

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[1] G. Ceder, (1998): *Science* **280**, 1099-1100.

When Pantelides indicated that time-dependent density functional theory could address some outstanding problems, Millis' response was that the quality of these computations is yet to be fully established. Millis then briefly described dynamical mean field theory as an example of an approach that may hold promise for dealing with dynamical situations. This approach has had limited but encouraging success dealing with simplified model systems of the colossal magnetoresistive materials. The two theoretical talks served to emphasize both the promise and the practical difficulties of accurate theoretical materials property prediction in systems at practical temperatures and real-world situations.

Design and manufacturing engineers found such trends to be of minimal value for designing reliability and improving manufacturability. Examples cited from the semiconductor industry showed manufacturing problems solved by empirically and laboriously developing algorithmic solutions for each specific process. A general consensus was that manufacturing engineers did not have confidence in the near term development of robust theoretical models for manufacturing but did look for and find useful fundamental inputs that helped them improve parameterized process characterization.

Manufacturing with rapid prototyping was highlighted in several talks. A principal incentive for this work filled a need to make complex shapes in hard materials (ceramics) while minimizing machining. Another consideration was the opportunity to manufacture parts with precision and complex geometries layer by layer. These are either impossible or very impractical to make by other methods.

Participants were challenged by the workshop objective to manufacture reliably at smaller and smaller scales. Several speakers, Chason and Hofmeister in particular, emphasized the importance of in-situ diagnostics for online processing control. This would seem to be of increasing importance for higher resolution and smaller scale part sizes. It was evident that spin-offs from new research in this area would also have payoffs at larger part dimensions.

SOLID FREEFORM FABRICATION - MACROSCOPIC OBJECTS TO FINE FEATURED COMPONENTS

Joseph Beaman
University of Texas, Austin

This presentation focuses on present capabilities and future challenges in laser based freeform fabrication of fine feature objects, with particular emphasis on selective laser sintering and selective area gas phase deposition. These processes have demonstrated capability of fabricating features on the order of a few millimeters in a number of materials. Process development efforts are presently under way to extend geometric and compositional fine feature capability in monolithic as well as multi-material components down to the microscale.

The ability to make fine featured components with feature sizes on the order of a few millimeters down to a few hundred microns is influenced by several factors. The most important factors affecting fine feature capability in laser based freeform fabrication processes are powder particle size, focused beam diameter, beam positioning resolution as well as powder layer thickness. In addition, heat transfer effects at part boundaries cause thermal sintering growth that results in alteration of part dimensions and possibly part distortion. Another challenge posed by powder based laser fabrication of fine featured components is the removal of unprocessed powder from features such as crevices and holes without affecting feature geometry.

JOSEPH BEAMAN

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   My research includes advanced manufacturing methods such as solid freeform fabrication and, systems modeling and control, an example being special melting technologies such as vacuum arc remelting and electroslag remelting. Areas of study include laser powder interactions, machine design and process control, computational geometry, physical modeling, structure/property characterization and advanced materials processing.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   Critical assumptions are that a material will interact with laser radiation and undergo a structure/property transformation (e.g., phase change), that the material can be processed to a desired geometry, microstructure and mechanical properties. One limitation of solid freeform fabrication (SFF) is the minimum feature size that can be successfully created, which is a function of the powder particle size, the wavelength and focused diameter of the laser beam, and the minimum powder layer thickness.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   An example of the production of Magnesium-Silicon Carbide metal matrix composite components by laser sintering that meet material property and chemistry specifications of conventionally processed material.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   Carl R. Deckard and Joseph J. Beaman, Solid Freeform Fabrication and Selective Powder Sintering, Proceedings of the 15^{th} North American Manufacturing Research Conference Proceedings, SME, 1987, pp. 636-640.

   1990 Solid Freeform Fabrication Symposium Proceedings, The University of Texas at Austin.

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   SFF technologies were initially developed for rapid prototyping, design visualization and testing in surrogate materials. Lately, there has been tremendous growth in rapid prototype tooling as well as fabrication of functional, fully dense, low volume or one of a kind materials having structure and properties equivalent to or better than conventionally processed material. Another burgeoning area within SFF is the development, design and fabrication of components with discrete or functionally graded material interfaces.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   Some of the key issues that should be addressed are the impact SFF technologies will have in the future by allowing designers to design region specific tailored material properties.

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Freeforming and Biomimetic Materials

Paul Calvert
University of Arizona

Freeform fabrication methods allow parts to be built layer-by-layer under the control of a 3D CAD model. Originally the materials were weak and could only be considered as prototypes but their mechanical properties are improving rapidly. This family of techniques allows multiple materials to be incorporated into a single monolithic part. Functional gradients, local reinforcement, porosity and local orientation can all be used to optimize the mechanical response of a part. It is less clear how to predict the optimum, especially for mobile systems subjected to dynamic loading.

The same methods can be used to incorporate electrical and optical components into freeformed parts, but combined deposition methods will be needed to achieve fine resolution of active components and rapid building of bulk objects. The apparent advantages of this approach include ruggedness and the ability to build 3D circuits.

Since most biological systems are also built layer-by-layer, we can look to plants and animals as a guide to what should be achievable by freeforming.

PAUL CALVERT

<u>SPEAKER QUESTIONAIRE</u>

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   I work on biomimetic materials and solid freeform fabrication. Biological materials and systems have many features that would be very valuable if we could reproduce them in a synthetic structure. since most biological materials grow layer-by-layer, layerwise processing methods are an obvious tool to allow us to build biomimetic materials.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   One outstanding feature of biological systems is their toughness, at all scales from the whole animal to the individual materials. They are obviously built for use under conditions where minor impacts are common. However, looking at the structure of bone or tooth, we cannot really see where the toughness comes from.

   Animals also have complex 3D systems of nerves and capillaries. Freeforming can now produce linewidths of 0.1mm but not routinely in multiple materials, such as we would need to build a nervous system into an artificial animal. Another tenfold improvement in resolution would have a tremendous effect.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   We have been building composites with locally controlled fiber alignment and with multiple layers of different materials to try to improve mechanical properties. We are working on metal-ceramic graded parts to provide high toughness with good wear resistance. Better tools for strength and toughness prediction in multi-material structures would help greatly.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   Griffith, M.L. and Holloran, J.W., "Freeform Fabrication of Ceramics Via Stereoithography", J. Am. Ceram. Soc. 79, 2601-2608, 1996.

   Sigmund, O., Torquato, S. and Aksay, I.A., "On the Design of 1-3 Piezocomposites Using Topology Optimization:, Journal of Materials Research 13, 1038-1048, 1998.

   Griffith, L. G., Wu, B., Cima, M. J., Powers, M. J., Chaignaud, B. and Vacanti, J. P. "In Vitro Organogenesis of Liver Tissue" in Bioartificial Organs (eds. A. Prokop, Hunkeler, D. & Cherrington, A.D.) (NY Academy of Sciences, New York, 1997) pp. 382-397.

Dimos, D., Yang, P., Garino, T. J., Raymond, M.V. and Rodriguez, M.A., "A Direct-write Fabrication of Integrated, Multi-layer Ceramic Components" in Solid Freeform Fabrication Proceedings (eds. Bourell, D.L., Beaman, J.J., Crawford, R.H., Marcus, H.L. & Barlow, J.W.) (U. Texas, Austin, 1997) pp. 33-40

P. Calvert, R. Crockett, "Chemical Solid Free-form Fabrication: Making Shapes Without Molds" Chem. Mater. 9 650-663 (1997)

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   Our interest is expanding from structural materials to include freeformed batteries and sensor systems. We can form actuators, but only from soft gels. Ultimately I see layerwise processing as providing a way to form whole systems which are currently assembled from any parts.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   I would like to understand more about how to optimize toughness in a composite structure, such as a bone. I am interested in the possibility of combinations of lithography and writing methods for large structures with fine internal details. There are many aspects of the freeforming processes that need modeling on the micron scale.

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In Situ Diagnostics for Thin Film and Surface Processing

Eric Chason
Brown University

In situ diagnostics are likely to play an increasingly important role in the development of advanced manufacturing methods. This role will encompass both research into new materials and methods, as well as a more active part in the actual processing environment. In research, advanced diagnostics are critical for validating computational models. This validation is necessary to reliably extend the models beyond being descriptive of well-known phenomena to being predictive of new phenomena. On the factory floor, diagnostics will allow us to design machines with a greater awareness of their state in order to increase reliability (e.g., by staying within tighter specifications) and reduce down-time (e.g., to predict the need for service). Such awareness is critical for agile manufacturing where a machine may be expected to rapidly change the material it is producing instead of working with a single laboriously-optimized single set of parameters. In this case, diagnostics are essential to rapidly optimize a new set of process parameters as well as to ensure that the machine stays within its optimal range.

In this talk, I will discuss several in situ diagnostics that we have developed for measuring the kinetics of surface and thin film processing. An important aspect of these techniques is that they are compatible with multiple processing environments:

1) Multi-beam Optical Stress Sensor (MOSS) – MOSS is an optical technique for measuring stress in thin films by measuring the curvature of the wafer. By using an array of parallel beams (instead of moving the beam or the sample), the curvature can be measured with no moving parts, significantly reducing the effect of sample vibration. We give examples of the use of this technique in several areas: strained layer semiconductor heteroepitaxy, metal polycrystalline films, GaN CVD growth, sputter deposition and pulsed laser deposition of hard coatings.

2) Light Scattering Spectroscopy (LiSSP) – LiSSP is a technique that was developed for measuring the power spectral density of the surface morphology during growth or sputter-etching. By using a broad-band Xe arc lamp source and a solid-state spectrometer, the full spectrum of scattered light is measured during processing without having to move the sample, the source or the detector. LiSSP has been applied to the kinetics of island growth and self assembly in SiGe/Si(001) and to the formation and decay of sputter-induced ripples on semiconductor and amorphous surfaces.

3) Energy Dispersive X-Ray Reflectivity (EDXRR) – X-ray reflectivity is a technique for measuring thin film roughness and layer thickness non-destructively. By using energy dispersive detection and a broad-band x-ray source, the reflectivity spectrum is obtained more rapidly than by conventional angle scanning means. Full XRR spectra have been obtained in only 20 x from metal films on oxidized Si. This rapid acquisition makes it possible to monitor the evolution of the surface during growth (by evaporation or CVD) and sputter etching, as well as to look at reactions at buried interfaces during annealing.

ERIC CHASON
DIVISION OF ENGINEERING, BROWN UNIVERSITY

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   My main interest is the evolution of thin films and surfaces during processing. A major aspect of this is the development of real-time, in situ diagnostics that enable us to monitor thin film kinetic processes while they occur (e.g., multibeam optical stress sensor, light scattering spectroscopy, energy-dispersive X-ray reflectivity). These techniques are currently being used to study the interaction of stress and morphology during semiconductor heteroepitaxy and during poly-crystalline metal film growth. Other recent studies include CVD growth kinetics, ion-assisted deposition processes, thin film interfacial reactions and Monte Carlo simulations of film growth and sputtering

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   The primary limitations of these techniques are that they are spatially averaging or diffraction based. For a full picture, they are best complemented by ex situ imaging techniques. However, the kinetic information provided by these real-time probes enables us to focus on where these ex situ studies should be done.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   The most significant recent success of this work has been understanding the interaction between stress and surface morphology during SiGe heteroepitaxy. By simultaneously measuring the film stress and the island density during growth, we have been able to quantitatively study the kinetics and energetics of island formation. These studies indicate that it is not sufficient to consider the elastic energy of the islands in isolation. The elastic interaction between adjacent islands also affects its evolution, leading to self-assembly of island arrays, changes in island shape and accelerated coarsening kinetics. Measurements have also been performed during GaN CVD and during TiN sputter deposition to measure the stress evolution during growth.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

J. A. Floro, G. A. Lucadomo, E. Chason, L. B. Freund, M. Sinclair, R. D. Twesten, R. Q. Hwang (1998), "SiGe island shape transitions induced by elastic repulsion," *Physical Review Letters* **80**, 4717.

J. A. Floro, E. Chason, M. Sinclair, G. A. Lucadomo, L. B. Freund (1998), "Dynamic self-organization of strained islands during SiGe epitaxial growth," *Applied Physics Letters* **73,** 951.

E. Chason, M. B. Sinclair, J. A. Floro, J. A. Hunter and R. Q. Hwang (1998), "Spectroscopic light scattering for real time measurements of thin film and island evolution," *Applied Physics Letters* **72**, 3276.

E. Chason and T.M. Mayer (1997), “Thin Film and Surface Characterization using Specular X-ray Reflectivity,” *CRC Critical Reviews in Materials and Solid State Science* **22**, 1.

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

I think that in situ process diagnostics will be an essential component of the future manufacturing environment. They are an efficient way of reducing the cycle time between design and process optimization. Techniques that are currently used as research tools can be transferred to the manufacturing environment if they are robust and easily interpreted. For instance, the stress monitoring technique we developed has been used to monitor stress evolution on the walls of a commercial sputtering chamber in real time. Enhanced monitoring during processing can also reduce the need for testing after production to see if the design specifications have been achieved.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

Tremendous advances in computational capabilities are making it possible to predict the properties of new materials. I think that it is critical that we have good experimental validation of these models to make sure that they are capturing all the essential physics. In addition, I think that there is still a big gap between being able to predict the properties of a material and designing the process for producing that material. Integrating modeling into the full cycle from designing to prototyping and then to manufacturing is still a big challenge.

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FUNDAMENTAL PHYSICAL CONSIDERATIONS IN MESOSCALE PROCESSING OF MATERIALS

Leonard C. Feldman
Vanderbilt University

Materials processing on the mesoscale has its fundamental roots in the thermodynamics of solids and the kinetics which govern the rates. Many issues of direct interest deal with interfaces of dissimilar materials. These concerns start with basic morphology considerations, extend to new phase formation and solid state reactivity and include a variety of other major materials phenomena such as surface diffusivity, grain boundry diffusion, amorphicity vs crystallinity, and a variety of complex phenomena which control the properties of the interface. This talk will review our understanding of some of these processes. The relationship to long term materials reliability will be noted.

L. C. FELDMAN

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   1. Experimental studies of interfacial properties: dielectrics on semiconductors, metals on organics, interfaces of nanocrystals.
   2. Fabrication of structures via finely focused ion beams, metallic nanocrystals, semiconductor nanocrystals, evolution of morphology with nanoscale structures.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   Limitations: 1) Quantitative analysis of non-planar structures
   2) Role of defects and defect agglomeration
   3) Near surface diffusion coefficients
   4) Use of FFIB for manufacturing due to slow "writing" speeds

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   1. Numerous examples of hardening, corrosion reduction, enhanced oxidation, phase changes and new materials fabrication via ion implantation.
   2. Controlled morphology

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   M. Zinke-Allmany, et al, "Surface Science Reports", 16, 1992 "Clustering on Surfaces".
   K.J. Gabriel, Sci. Am., 260, 118 (1995) "Engineering Microscopic Machines"
   K. Tu, et al, "Electronic Thin Film Science", MacMillan, (1992)

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   No comment.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   1. Interplay of modeling and manufacturing. In particular, need theorists to cite missing "data" that would permit more full scale modeling.

   2. Handling of amorphous materials.

Compliant Mechanism Based Manipulator Design For Micromanipulation and Microassembly

Michael Goldfarb
Vanderbilt University

Significant microscope technology exists for the purpose of observing small-scale environments. Physical interaction with such environments, however, remains severely limited by the mismatch between the small-scale environments and the limitations of machine dexterity imposed by conventional machine design. Specifically, insufficient technology exists to handle and assemble small (e.g., MEMS) parts, which is a significant limitation in the development of multi-component MEMS devices. Unlike conventional manipulator design, a compliant mechanism design enables the development of precision manipulators without the backlash and Coulomb friction that impede small-scale position and especially force control. A compliant mechanism approach to precision manipulator design can provide significant workspace and robust closed-loop stability in high (and variable) impedance environments, and thus can eliminate the inconsistency that currently exists between the available technology for observing small-scale environments and the technology for manipulating it.

MICHAEL GOLDFARB
VANDERBILT UNIVERSITY

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   My research focuses on the design and control of precision manipulators for microassembly and micromanipulation. In particular, the work involves the design of compliant mechanism based manipulators for precision position and force control.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   My work is a design approach and not a method per se.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   I'm not sure this question is relevant to my research.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   Goldfarb, M. and Speich, J.E. A Well-Behaved Revolute Joint for Compliant Mechanism Design. *ASME Journal of Mechanical Design*, In press.

   Goldfarb, M. and Celanovic, N. A Flexure-Based Gripper for Small-Scale Manipulation. *Robotica*, In press.

   Goldfarb, M. Similarity and Invariance in Scaled Bilateral Telemanipulation. *ASME Journal of Dynamic Systems, Measurement, and Control*, In press, to appear March 1999.

   Goldfarb, M. and Sirithanapipat, T. The Effect of Actuator Saturation on the Performance of PD-Controlled Servo Systems. *Journal of Mechatronics*, In press.

   Goldfarb, M. and Celanovic, N. Modeling Piezoelectric Stack Actuators for Control of Micromanipulation. *IEEE Control Systems Magazine*, vol. 17, no. 3, pp. 69-79, 1997.

   Goldfarb, M. and Celanovic, N. A Lumped-Parameter Electromechanical Model for Describing the Nonlinear Behavior of Piezoelectric Actuators. *ASME Journal of Dynamic Systems, Measurement, and Control*, vol. 119, no. 3, pp. 478-485, 1997.

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   Micromanipulation and microassembly.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   Microassembly and micromanipulation would be relevant topics in a "Factory After Next" workshop.

FINITE ELEMENT METHODS FOR MODELING QUANTUM PHENOMENA AND ELECTRONIC/MECHANICAL COUPLING IN THIN FILM STRUCTURES

H.T. Johnson, R. Phillips, and L.B. Freund
Brown University

Thin film semiconductor structures containing defects or consisting of lattice mismatched materials are often highly strained. The strain in these complex, nanometer scale structures can be very nonuniform. Because of the possible applications of the structures, it is important to understand the effects of the mechanics on the quantum and electronic behavior. Experimental evidence suggests that the coupling of strain and quantum or electronic effects is significant, but there is a need for continuum based modeling methods for these coupled boundary value problems. Two such techniques are presented here.

A continuum finite element technique for studying quantum mechanical confinement in strained structures is discussed first. In this model, strain effects are treated as a *perturbation* on undeformed electronic properties. The linear elastic strain in a quantum dot or wire is first determined by a finite element calculation. A strain-induced potential field that perturbs the energy band structure in the body is then determined from deformation potential theory. The time-independent Schrodinger equation containing the nonuniform potential field is then solved, also by means of the finite element method. The solution consists of the wavefunctions and energies of confined states in the structure. The first example discussed is the case of a Ge pyramid shaped island quantum dot on a Si substrate; the effects of island size on confinement energies are examined. Then, in order to make contact with experimental transport data, several Si_xGe_{1-x} resonant tunneling quantum devices are analyzed.

Second, a mixed atomistic/continuum technique is formulated and used to solve boundary value problems with fully coupled electronic and mechanical material properties. The technique is implemented by means of a standard structural mechanics finite element package, and significant savings in computational cost are achieved over fully atomistic calculations. For each increment of load applied, within each element in the mesh, tight binding atomistic calculations are made for energy, stress, and elastic constants. This information is used by the finite element program to solve for equilibrium nodal displacements to be used at the beginning of the next load increment. Because the tight binding calculation is based on quantum mechanics, electronic properties can also be extracted at the element level. The technique is demonstrated by examining several simple plane strain boundary value problems for coherently strained silicon. Improvements in the formulation which are under development are also discussed, including the ability to model elements containing atoms in *nonuniform* environments.

The relative merits and the limitations of these two techniques for characterizing submicron semiconductor structures are discussed. The continuum technique is compared to full atomistic analyses that have been reported for similar problems, and prospects and challenges for the development of the mixed atomistic/continuum method are discussed. Possible extensions of the mixed atomistic/continuum technique, based on developments in atomistic and mixed techniques, include studies of defects, surfaces, and bimaterial interfaces.

H.T. JOHNSON

<u>SPEAKER QUESTIONAIRE</u>

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   My current research is on two techniques for studying strain effects on quantum phenomena and electronic properties in semiconductor structures. The first method is a continuum finite element technique in which strain is treated as a perturbation to quantum mechanical behavior in structures. The second technique is a mixed atomistic/continuum approach in which electronic and mechanical properties of a strained body are treated as fully coupled.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   The modeling methods I use are based on the finite element method, so there is some numerical approximation involved. Also, the quantum mechanical basis of the techniques is somewhat limited. The continuum approach relies on perturbation theory, and the atomistic/continuum technique depends on an empirical tight binding parameterization.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   Much of my work focuses in some ways on electronic properties. However, the continuum technique has been used to study transport in quantum devices, and the mixed atomistic/continuum technique is used to determine mechanical structure in strained bodies, based on atomistically derived mechanical properties that reflect the quantum mechanics of bonding.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   A. Zunger, MRS Bull, **23** 15, (1998)
   M. Grundmann, O. Stier, D. Bimberg, Phys. Rev. B **52**, 11969 (1995)
   H.T. Johnson, L.B. Fruend, C.D. Akyuz, A. Zaslavsky, J. Appl. Phys. **84**, 3714 (1998)
   E.B. Tadmor, M. Ortiz, R. Phillips, Phil. Mag. A **73**, 1529 (1996)
   W.A. Harrison, Electronic Structure and the Properties of Solids, 2^{nd} Ed. (Dover Publications, New York, (1989)

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   The continuum technique is useful for predicting the practical value of various configurations, geometries, and compositions for quantum dots and wires. The mixed atomistic/continuum technique is expected to be used to predict coupling of properties in structures that feature nonuniform geometries, lattice mismatch, atomic scale defects, and bimaterial interfaces.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   I am interested in thinking about ways that theory and computation can be used to guide experimental work, and about ways that experimental research can be used to guide actual processing and manufacturing methods. From a modeling perspective, it is interesting to consider the implications of moving to smaller length scales. Atomistic methods become more important, and material properties become more challenging to model and predict.

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PRACTICAL CONSIDERATIONS FOR DESIGNING ULTRA-LARGE SOFTWARE SYSTEMS

Gabor Karsai
Institute for Software-Integrated Systems
Vanderbilt University

It is a well-known observation that systems (of systems) are getting more difficult to understand, design, build, operate and evolve. Arguably, some of this complexity can be attributed to that fact that a significant portion of the sophistication of military and industrial systems is derived from a software component. Several "software glitches" have been observed in the recent past where the complex interactions between the software and its environment lead to undesired behavior, occasionally damage to the physical components of a system.

Systems that heavily rely on software to accomplish their mission can exhibit very complex behaviors. As the complexity of the software grows, the potential paths of interaction among the software components, and the effect of these interactions on the physical components of the system grows even more complex. Currently we don't have good development processes to mitigate these interactions. Software has to satisfy multiple, often contradictory, functional and non-functional requirements. Typically the requirements cut across a large number of software components, and it is extremely hard to predict the effect of a design change with respect to the requirements. The software is often placed into a physical environment, but this "coupling" between the software component and the physical world is often overlooked in the software development process.

We argue for an integrated approach and related support technology for addressing issues arising in large-scale software development, especially when the software must operate in a changing environment. Software, its environment, and the interaction between them must be explicitly modeled, and the models should capture all relevant aspects of the design. Hardware and software design processes need to be integrated, as well as system-level design tools are needed that allow tracking down of complex interactions among components. Synthesis and design verification approaches (as championed mostly in the hardware, and somewhat in the software) should be used whenever possible. Components and component integration mechanisms should be used uniformly, and dependencies among components should be explicitly formulated and documented.

To summarize, models are needed to capture what we know, synthesis should be used to generate the "non-interesting" parts of software, and integration of hardware, software, and system design is necessary to tackle complex requirements.

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ATOMIC EFFECTS IN BRITTLE FRACTURE

Michael Marder
Department of Physics and Center for Nonlinear Dynamics
The University of Texas
Austin TX, 78705

Ideal brittle fracture is a connected set of qualitative phenomena associated with the failure of brittle crystals at zero temperature. In particular

- A range of initial conditions produces cracks moving in atomically perfect steady states, leaving behind perfectly flat fracture surfaces.
- Constant velocity crack motion below a lower critical velocity is forbidden.
- Above an upper critical velocity, steady states become unstable, and produce a wide variety of complex energy-consuming structures.

This class of phenomena clearly emerges from a collection of models which follow the fracture process down from the macroscopic to microscopic scales, and can be solved analytically. However, it has not been clear whether the behavior of these models followed from unrealistic features, such as the snapping bond potentials that allowed analytical solution, or whether the results were general.

I will present evidence from molecular dynamics simulations that the results are in fact general. They appear in three-dimensional molecular dynamics simulations of silicon and silica that employ medium-range forces between atoms and three-body interactions. The realistic simulations are capable of some interesting new dynamical behavior, including stable multiply-periodic states, that happen not to occur for the analytically solvable models. Otherwise they are qualitatively identical. Data from laboratory experiments in silicon will also be presented.

MICHAEL MARDER
THE UNIVERSITY OF TEXAS

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   On brittle fracture:
   Analytical solutions of simple models
   Massively parallel molecular dynamics
   Laboratory experiments

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   Knowledge of proper force laws between atoms is right now the limiting step. The concept of "force laws" may not be adequate.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   We can predict many features of crack behavior – initiation, velocity, instabilities, and compare directly with experiment. Most work in single crystal silicon.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   - L. Ben Freund's "Dynamic Fracture Mechanics"
   - Origin of create tip instabilities" an article I published in 1995 in Journal of Mechanics and Physics of Solids
   - Texts on condensed matter physics and references on interatomic potentials and density functional theory

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   Fracture behavior of silicon is a test case of basic importance, but I do not yet know of many applications.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   I would appreciate an opportunity to move past the hype that can surround computational materials, and look at what we really can or cannot achieve.

NOVEL JOINING TECHNIQUES FOR ADVANCED MATERIALS

David L. Olson
Colorado School of Mines

Advanced materials are based on engineered microstructures to achieve properties. The joining of these materials into a technical assembly requires techniques that do not take the parent material into the liquid state and do not alter its microstructure. The challenges in fabricating the leading edge technical assemblies will be discussed. Novel joining techniques will be introduced which satisfy some, if not all, of the joining process requirements.

DAVID OLSON

COLORADO SCHOOL OF MINES

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

    - Welding and joining research
    - Thin film microstructure evolution
    - Reactive metals (alkali, alkaline earths, actinides, and rare earths)

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

    Cold and warm joining
    - Surface preparation
    - Applied load
    - Coatings

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

    - Any assembly made up of dissimilar alloys
    - Weapons

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

    1. V. Sabather, G.R. Edwards and C.E. Cross, Kinetic Study of Low-Temperature Transient Liquid Phase Joining of an Aluminum-SiC Composite, Met. Trans. 25A(12) p-2705-2714 (1994)
    2. M. O'Brien, C.R. Rice and D.L. Olson, High Strength Diffusion Welding of Silver Coated Bare Metals, Welding J. 65(1) pp 25-27 (1976)
    3. R.A. Nichting, D.L. Olson and G.R. Edwards, J Mat Eng & Perf. 1 (1) pp35-44 (1992)

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

    Essential for advancement in material used in advanced technical assemblies.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

    Cold or warm joining requires accurate alignment and application of force, knowledge of theoretical strengths for dissimilar metal joints, and a very difficult inspection problem.

COMPUTATIONAL MATERIALS SCIENCE – FROM ATOMS TO MACROSCOPIC PROPERTIES

Sokrates T. Pantelides

Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235

In the industrial world, decisions are made about materials science by considering the ultimate function of the material in the final product, processing requirements, manufacturing requirements, the resistance to failure during use, and cost. Engineers need information about the material that can be used to design and develop the manufacturing process and assess the ultimate reliability of the product. Much of that information is usually gathered empirically. In recent years, however, atomic-scale theory has made enormous strides in its ability to provide information that is useful and often indispensable for product development. The translation of atomic-scale information to process and product developers can take many different routes. This talk describes a few examples where distinctly different routes are appropriate.

Case I. This is an example where atomic-scale information is used directly to modify materials processing. GaN is a material that is at the forefront of blue-green optoelectronic devices. However, wide commercial use is still impeded by low p-type conductivity. P-type doping is usually achieved by incorporating Mg during growth. It has been found that everpresent H passivates substitutional Mg and is subsequently removed by annealing. There is evidence, however, that only a fraction of Mg is activated and vibrational signatures suggest the possibility of defect complexes tying up Mg in inactive forms. Through first-principles calculations[1] we identified several defect complexes involving substitutional and interstitial Mg and H. The results led us to suggest that, after growth and prior to annealing the material to remove H, one should first anneal at moderate temperatures in an H atmosphere to get more H in! This process would convert the undesirable defect complexes into more benign forms such as passivated substitutional Mg. After this step, annealing in an N_2 atmosphere at higher temperature as usual to remove the H would produce higher doping levels. The idea is currently being tested.

Case II. This is an example of going from the atomic scale to an intermediate “mesoscopic” scale and then to the processing world. Two examples will be presented: Oxygen precipitation, where first-principles calculations[2] identified the relevant atomic-scale pathways; Hydrogen precipitation, where first-principles calculations identified the pathways that lead to the formation of planar platelets that ultimately underlie the so-called smart-cut process for forming silicon-on-insulator (SOI) structures[3]. In all such cases of precipitation, once the atomic-scale processes are identifies one must perform Monte-Carlo calculations to establish parameters for controlling the form and behavior of the precipitates at the mesoscopic scale.

Case III. This is an example where from the atomic scale one goes to the mesoscopic scale and describes dynamical processes in terms of fluxes and densities of defects that then are related to macroscopic stress and strain fields. Particular examples will be given of void growth under anisotropic stress and under external currents. The latter is an example of electromigration that has been a persistent problem in microelectronics and is handled with empirical rules[4].

1. F. Reboredo and S. T. Pantelides, “Novel Defect Complexes and Their Role in P-type Doping of GaN”, Phys. Rev. Lett. 82, 1887 (1999).

2. M. Ramamoorthy and S. T. Pantelides, "Atomic Dynamics during Silicon Oxidation and the Nature of Defects at the Si-SiO_2 Interface", Appl. Phys. Lett., June 1999, in press.

3. F. Reboredo, M. Ferconi and S. T. Pantelides, "Theory of the Nucleation, Growth, and Structure of Hydrogen Platelets in Crystalline Silicon", Phys. Rev. Lett., June 1999, in press.

4. S. T. Pantelides, D. Maroudas, and D. B. Laks, "Defects in Heterogeneous Solids -- From Micro to Macro Physics", Mater. Sci. Forum 143, 1(1994).

SOKRATES T. PANTELIDES
VANDERBILT UNIVERSITY

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   First-principles density functional simulations of atomic-scale structures and dynamics in materials – interactions of intense radiation with materials (selective processing) – nanodevices – connections to mesoscopic and macroscopic length scales.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   Quantum mechanics – density functional theory, local density approx. for exchange-correlation.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   - Predicted segregation of imperitios in grain boundaries in selected columns as ordered chains – verified by atomic-resolution TEM

   - Precipatation of O in Si, H in Si in form of platelets

   - Void evolution and creep in metals.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   Hohenberg and Kohn (1964)
   Car and Parrinello (1985)
   Bernliolc, Lipari and Pantelides (1979)

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   Direct connections to industrial modeling.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   Connecting basic research to industrial modeling.

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NUCLEATION CONTROL IN MATERIALS SYNTHESIS AND PROCESSING REACTIONS

Professor J. H. Perepezko
University of Wisconsin-Madison

Microstructure control is a key objective of most forms of materials processing. Often, the initial stage of processing is controlled by a nucleation step that sets the product phase number density, size scale and structure in the overall microstructure. In fact, the development of supersaturated solutions or undercooled liquids is closely linked to nucleation control. A kinetic competition is also a common feature of nucleation-controlled reactions and presents a challenge for analysis since only the victor of the competition survives for observation. At the same time, it is important to recognize that nucleation is a probabilistic enterprise. This characteristic can be exploited in experiments that expose a kinetic transition between competing nucleation reactions to allow for an assessment of the relative kinetic rates during processing. For heterogeneous nucleation, new experimental strategies can allow for the identification of active nucleation sites and the hierarchy of potency for some solidification reactions. This insight on catalysis behavior has been applied to model the evolution of high primary phase grain densities during rapid freezing of surface coatings as well as nanocrystal development during devitrification reactions. In the latter case, multicomponent alloying effects resulting from unequal component diffusivities have been used to implement a kinetic stabilization strategy for enhanced thermal stability of the nanocrystalline structure. The identification of nucleation control has been extended recently to the initial stage of interdiffusion reactions involving the formation of intermediate phases such as those that control the stability of composites and occur in many coating applications. For these studies, multilayer samples are most effective in emphasizing the nucleation stage of both stable and metastable phases for kinetic measurements. Some of the basic characteristics of nucleation control are illustrated by experimental observations and analysis models that highlight the current understanding and outstanding issues in novel materials synthesis reactions.

J. H. PEREPEZKO
UNIVERSITY OF WISCONSIN-MADISON

<u>SPEAKER QUESTIONAIRE</u>

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   My work involves the study of the synthesis and processing fundamentals governing the formation of novel non-equilibrium structures and their evolution and stability during post synthesis treatments. A primary focus of the work is directed toward solidification processing methods, especially under nucleation control conditions, in which structure synthesis at high undercooling and high rates is achieved by removing nucleants from the melt and/or subjecting the liquid to a high cooling rate. A variety of alloy structures is examined by thermodynamic and structural characterization methods. Often, nanoscale structures are of key importance in the work. A recent emphasis is on amorphous Al alloys where controlled devitrification can yield high strength levels with high thermal stability. The key issue in maximizing strength is to control the nanocrystal particle density which is being addressed by a new theoretical model for multicomponent crystallization and by crystallization catalysis experimental strategies.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   The critical assumptions often relate to the extension of existing, essentially classical methods of thermodynamics and kinetics analysis that were developed to treat macroscopic scale processes under steady state conditions. The predictions from these methods for nanoscale structures and synthesis under non-equilibrium, non-steady state conditions are uncertain. The development of appropriate thermodynamic and kinetic models and the formulation of critical tests for the models are also important. In addition, many of the most interesting structures involved in nanocrystalline and bulk amorphous systems require multicomponent alloys for synthesis. A key limitation is the scarce experimental database of thermodynamics and diffusion kinetics measurements which are essential for even an approximate analysis of multicomponent behavior.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   There are several examples that can be cited, but in each case the limitation due to lack of experimental measurements of key properties is apparent. In the analysis, the deficiency is often addressed by using an experimental result to “calibrate” the model. This approach ensures agreement between the analysis and the observations, but the reliability of prediction outside of the "calibration” range is uncertain. some brief cases are listed below.

   a) Overall modeling of the grain structure (i.e., size, number and shape) developed during solidification where nucleation and growth kinetics together with heat and fluid flow are treated.
   b) Heat treatment response of steels.
   c) Analysis of surface microstructure during laser surface melting of eutectic alloys.
   d) Modeling of devitrification reactions leading to nanocrystal synthesis from amorphous alloys.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

a) M. Rappaz, Int. Mat. Rev., 34,93 (1989)
b) W.J. Boettinger and J.H. Perepezko, “Rapidly Solidified Alloys: Processes, Structures, Properties, Applications” H.H. Liebermann, ed. (Marcel Dekker, N.Y.) 17 (1993)
c) J.H. Perepezko and M.J. Uttormark, Met. Mat. Trans. 27A, 533 (1996)
d) M. Grernaud, D.R. Allen, M. Rappaz and J.HJ. Perepezko, Acta Mater., 44, 2669 (1996)
e) D.R. Allen, J.C. Foley and J.H. Perepezko, Acta Mater., 46, 431 (1998)
f) A. Inoue, Mat. Trans. JIM, 36, 866 (1995)
g) A. Makino, A. Inoue and T. Masumoto, Mat. Trans., JIM, 36, 924 (1995)
h) G. Olson, Science, 227, 1169 (1997)
i) D. Turnbull, Metall. Trans., 12A, 695 (1981)

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

In short-term it seems clear that the attention that nanocrystalline structures are receiving will result in a number of applications for structural and magnetic uses. Similarly, bulk metallic glasses should also yield some novel applications (e.g., low friction uses) that are just being identified.

Over the long-term, a fully predictive methodology is evolving that will include the capability to treat real materials with the complexity that is encountered in manufacturing.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

A central issue is to identify areas with outstanding questions relating to the fundamental understanding of materials behavior and properties. From a sound foundation of understanding, past experience has shown many times that appropriate processing strategies can be devised. Extending processing from a laboratory scale to an industrial scale of manufacturing and production is a huge step that is often determined or influenced by non-technical issues. The ARO mission and the impact of the programs are best served by maintaining a focus on basic understanding.

In spite of the general data limitation, there are some examples (e.g., steels) where the database is more complete. In this case, the thermodynamics analysis is now being coupled with kinetics models in a fully interactive and predictive mode. In complex multicomponent systems so-called first principles calculations are not reliable for providing the required thermodynamic and kinetics information. This gives strong support to the most urgent need for reliable, careful experimental measurements.

Another key issue relates to the proper understanding of materials behavior and processing so that relevant scaling relationships can be formulated to guide processing, analysis and prediction.

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TECHNOLOGY COMPUTER-AIDED DESIGN TOOLS AND THE SEMICONDUCTOR INDUSTRY

Ron Schrimpf
Vanderbilt University

Technology Computer-Aided Design (TCAD) simulation tools have revolutionized the design and manufacture of integrated circuits. TCAD tool suites include capability for simulating everything from the fabrication sequence through circuit-level performance. The typical levels of TCAD simulation are:

1. Process simulation tools use information such as times, temperatures, and lateral patterns to generate device structural information, such as doping profiles and film thicknesses.
2. Device simulation tools use the device structural information, along with bias conditions, to calculate the device current-voltage characteristics. Many internal quantities, such as electric field, potential, and carrier concentrations, are also accessible through device simulation. Many of these quantities cannot be measured directly in actual devices.
3. Parameter extraction tools are used to obtain compact-model parameters from the device current-voltage characteristics for use in circuit simulation.
4. Circuit simulators calculate the electrical behavior of multiple active devices that are connected together, along with passive components.

The semiconductor industry relies heavily on these tools because modern devices are so complex that it is extremely difficult (if not impossible) to design them solely with analytical models or through trial and error. In addition, the cost of a modern semiconductor fabrication facility may exceed $1 billion, so it is very important to get working products in a very short time. If TCAD tools are sufficiently accurate, they can reduce the development time significantly. The cost of conducting virtual "experiments" is much less than that of actually trying things in the lab, so there is more freedom to try new approaches.

As other types of manufacturing become more complex, miniaturized, and expensive, they will be driven to use analogous simulation tools. There may be some lessons from the experience of the semiconductor industry that can be used to benefit other types of advanced manufacturing. For example, it is essential that simulators predict trends correctly and allow calibration to experimental data. Models should be physically based in order to enhance predictivity. It is important that the simulator be able to provide results in real time, or close enough to it that the engineer can test multiple strategies, evaluate them, and modify his approach. A corollary of this is that there is never enough computing power available; the complexity of the simulation methodology always expands to consume the computer resources. Integration of different levels of simulation tools into a single framework is critical. In the semiconductor industry, TCAD tools can be used to examine the effect of a process change on circuit performance, with all of the simulation tools linked together. In the future, it will be important for a single tool suite to offer both electrical and mechanical simulation. Use of simulation tools that are standard industry-wide allows development of more powerful tools and transfer of information between organizations. These issues and others will be considered in this presentation. Some illustrative TCAD examples will be presented.

RON SCHRIMPF

VANDERBILT UNIVERSITY

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   I work in the area of semiconductor devices, particularly radiation effects and reliability. This includes simulation/model development, and experimental work.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   We are using models for very small devices that were developed for larger devices. Although it is possible to get good results if one understands the devices, efficient models for small devices will be needed.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   All of our work is related to electronic properties, but this includes the effects of radiation on these properties. Some of the devices we study are electro-optical devices.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   This book provides a general overview of TCAD tools: R.W. Dutton and Z. Yu, "Technology CAD: Computer Simulation of IC Processes and Devices, "Kluver Academic Publishers," Boston, 1993.

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   It's important to couple the electrical and mechanical simulations.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   1. Simulation framework, integration, and interface
   2. Model verification
   3. Computational efficiency
   4. Customized vs standard simulation tools

MECHANICAL TESTING AND PROPERTIES

W. N. Sharpe, Jr.
Department of Mechanical Engineering
The Johns Hopkins University
Baltimore, MD 21218

The new microelectromechanical systems (MEMS) have stimulated interest in the mechanical properties of materials on a very small size scale. Newly developed mechanical testing capabilities can accommodate specimens with minimum cross-section dimensions on the order of one micron; their length may be as small as 50 µm or so. The need to extend these test methods to smaller size scales is imminent with the possibilities of even smaller microdevices based on carbon nanotubes.

Mechanical properties of materials have traditionally been measured with the simple tension (or compression) test; the advantage being that the stress and strain states are uniform. Those values can be used for components with more complex stress states through the mature discipline of solid mechanics. There are three main challenges to tensile testing on this scale.

- Preparation and handling of the specimen -- it is not easy to pick up a specimen and put it in a set of grips.
- Friction in the load train – forces may be as small as a few milli-Newtons.
- Direct strain measurement on the specimen – measuring the overall displacement of a specimen can introduce errors.

We have developed techniques and procedures at Hopkins for tensile testing of thin-film polysilicon (1.5 µm thick) and thick-film electroplated nickel (100 µm thick). In each case, the width of the uniform gage section of the tensile specimen is similar to the thickness. The polysilicon specimens are deposited on a silicon wafer with one end fixed and the other free to be gripped with an electrostatic probe; therefore no friction exists between the moveable end of the specimen and the grip. The nickel specimens are 3 mm long and can be placed in a set of grips supported by a linear air bearing.

Strain is measured directly on these specimens with laser-based interferometry from reflective markers on the central gage section. For thin films, gold lines are deposited on the specimen surface; these are 20 µm side and 200 µm apart. Reflective indentations 20 µm square are placed in the nickel specimens with a diamond indenter. A low-power He-Ne laser shining on the markers produce reflected (diffracted) fringe patterns that move as the markers move apart upon force application. Those motions are monitored with linear diode arrays and a computer-controlled system to enable real-time strain measurement. These test systems are described in more detail in:

Sharpe, W. N., Jr., Yuan, B., Edwards, R. L., and Vaidyanathan, R., ‘‘Measurements of Young’s modulus, Poisson’s ratio, and Tensile Strength of Polysilicon’’, *Proceedings of the Tenth IEEE International Workshop on Microelectromechanical Systems*, Nagoya, Japan pp. 424-429 (1997).

Sharpe, W. N., Jr., LaVan, D. A. and Edwards R. L., ’’Mechanical Properties of LIGA-Deposited Nickel for MEMS Transducers’’, *Proceedings Transducers ‘97,* Chicago, IL, pp. 607-610, (1997).

W. N. SHARPE, JR.
DEPARTMENT OF MECHANICAL ENGINEERING
THE JOHNS HOPKINS UNIVERSITY

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   Tensile testing of small specimens, especially MEMS materials.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   Measurement of cross-section dimensions is difficult.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   Measurement of Young's modules and Poisson's ratio of polysilicon film.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   Sharpe, et at, "…..Polysilicon", Proc. 10th IEEE Int'l Workshop on MEMS, Naqoya, 1997, pp. 529-534

   Sharpe, et al, "…..Nickel…..", Transducers '97, Chicago, 1997, pp. 607-610

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   There is still a major lack of information on mechanical properties of the "new" materials used in MEMS.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   Mechanical properties are critical to design and life prediction.

THREE DIMENSIONAL MICROSTRUCTURALLY INDUCED DUCTILE AND BRITTLE MATERIAL FAILURE MODES IN METALLIC AND INTERMETALLIC MATERIALS

M.A. Zikry*

Department of Mechanical and Aerospace Engineering
North Carolina State University
Raleigh, NC 27695-7910

Ductile and brittle failure modes have been investigated for polycrystalline metallic and intermetallic materials separated by high angle random and coincident site-lattice grain boundaries. Thermo-mechanical deformation modes that result in ductile failure, such as shear-strain localization, or brittle failure, such as macroscopic crack formation and growth, have been characterized for quasi-static and dynamic loading conditions. Dislocation-density based analytical and computational constitutive formulations have been developed and coupled to mutiple-slip crystalline formulations to account for the effects of grain-boundary misorientations, dislocation densities, thermal and geometrical softening, and dislocation pile-ups on failure evolution.

* Currently, Associate Professor, North Carolina State University, Dept. of Mechanical and Aerospace Engineering,

M. A. ZIKRY
DEPARTMENT OF MECHANICAL AND AEROSPACE ENGINEERING
NORTH CAROLINA STATE UNIVERSITY

SPEAKER QUESTIONAIRE

1. Please provide a brief description, including the theoretical and/or experimental subjects and methods that characterizes your research.

   Computational predictive methods based on specialized finite-element that span mechanisms from the micro to the macro level. Dislocation density effects, crystal structure, and grain-boundary structure and morphology are coupled to failure initiation and evolution in polycrystalline aggregates subjected to three dimensional loading conditions and effects.

2. If possible, summarize in a few words the critical assumptions and limitations of the methods.

   Current limitations: Chemical effects are not coupled or linked to current formulations.

3. Can you offer brief examples of where these methods have been successfully used for structure/property prediction other than electronic behavior?

   - Texture Predictions
   - Failure Innitiation Prediction
   - Crack Growth/Direction Orientations

   These predictions are linked to the material's microstructure.

4. Please provide a brief list (1-3 at a minimum) of what you consider to be the key references in your field. (Include references to your own work when appropriate.)

   Nemat-Nasser and Horie, Micromechanics of Heterogeneous Materials, Elsevier Press.
   Havner, Crystalline Deformations, Cambridge Press.

5. General comments (relating the speculative potential uses, short-term/long-term potentials).

   Computations have to be performed on a scale that can be related to a scale commensurate with the macro level.

6. What are your initial impressions of the key issues that should be addressed in this workshop and their relationship to your current and past work?

   Relate computational predictions to failure, materials processing, manufacturing and component performance.

HIGH TEMPERATURE/PRESSURE THERMOPHYSICAL PROPERTY PREDICTION

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Thermal expansion approximated by contributions from a perfect crystal and its equilibrium high temperature/pressure defects. We demonstrate that the influence of thermal defects on high pressure thermal properties can be important. Thermophysical properties are interrelated and results for metals, and some structural ceramics are compared with available data and theoretical calculations.

Supported by the Army Research Office.

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ELECTRONIC AND MAGNETIC TECHNIQUES TO DETERMINE MICROSTRUCTURE AND PHASE STABILITY

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Basic to phase stability in alloys is the electronic structure and interactions in the metallic lattice. The Fermi energy level relative to the energy level of the Brillonin zone gap can be altered by solute additions thus with proper alloying promote specific phase transitions. Hall coefficient and more conveniently the thermoelectric power coefficient can be used to determine an approximate chemical potential for the conduction electrons in a metallic solid solution. Alloying effects on the filling of the d-states and f-states in the transition metals, rare earths and actinides can influence the preference of a specific crystal structures.

Magnetic measurements can be used to determine the susceptibility to phase formation, i.e. sigma phase formation in high alloyed ferrous materials, and to follow the hydrogen content in structural and hydrogen storage alloys. Electrical conductivity measurements can give some indication of structural features, primarily lattice defects such as grain boundaries, precipitation, etc. Combining these electrical and magnetic measurements into a 3D plot of thermoelectric properties, magnetic properties and electrical conductivity, the phase stability relative to a preferred microstructure zone can be identified and used with the electromagnetic techniques to monitor and control material processing and predict service behavior.

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HIGH RESOLUTION MEDIUM ENERGY ION BEAM ANALYSIS OF ULTRA-THIN FILMS*

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The characterization of ultra-thin films, those thinner than approximately 10 nm such as state-of-the-art gate oxides, is one of the most challenging problems of modern ion-beam analysis. In this presentation, we explore the strengths and limitations of time-of-flight medium energy backscattering and describe the physical processes that determine the resolution of elemental depth profiles. The primary determinants are uncertainty of ion path length, kinematic dispersion from the finite detector solid angle, straggling in the start foil, and variability of the start foil thickness. The first three of these have been considered in previous studies of time-of-flight spectrometer resolution, but foil non-uniformity has not been examined in detail. Using backscattering analysis and atomic force microscopy, we have measured the thickness and roughness of carbon start foils and found them to be larger than suggested by their nominal specifications. As a result, energy uncertainty introduced by foil non-uniformity has been found to be a critical factor in determining resolution. Using measured values of foil parameters and known geometric characteristics of our spectrometer, Monte Carlo simulations of backscattering spectra of SiO_2 thin films on Si substrates have been computed and found to reproduce well the experimentally observed system resolution of 1350 eV for 104 keV He. Additional simulations show that spectrometer design changes could reduce this value to about 1 keV at which point it is, for all practical purposes, optimum.

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SIMULATING MECHANICAL BEHAVIOR OF THERMAL BARRIER COATINGS VIA OOF*

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Knowing basic physical properties of plasma-sprayed thermal barrier coating (TBC's) is essential for design and reliability assessment of components using these coatings. In particular, mechanical properties, such as, elastic behavior and residual stresses, can have a strong influence on delamination behavior, and hence reliability. As mechanical properties are difficult to measure directly, an alternate stratagem is to develop numerical schemes for determining these properties from the complex microstructure of these materials. Such a computational tool, called OOF, has been under development at NIST. OOF, which stands for Object Oriented Finite element analysis, is a computational tool hat allows material scientist to simulate physical properties of complex microstructures from an image of that microstructure.

Computer simulations using OOF have been conducted on TBC's to elucidate the influence of microstructural features, such as, porosity, microcracks, interfacial surface roughness, and residual misfit strains, on mechanical behavior. OOF is used both for image analysis and for finite element simulations of thermoelastic behavior. First a digital image of a scanning electron micrograph, or a computer generated microstructure, is converted into finite element mesh, in which every feature of the microstructure has defined thermoelastic properties. Then a solver is used to determine the mechanical response of the finite element mesh to simulated boundary conditions and temperature changes. Results are presented that study the influence of microstructure, porosity and microcracks on anisotropic elastic behavior, and the influence of interfacial surface roughness on residual stress distributions. Recent extensions of OOF to incorporate fracture and damage accumulation are also discussed via simulations in polycrystalline brittle ceramics.

* Seminar presented to the U. S. Army Research Office on February 22, 1999.

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ARO/Vanderbilt
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